

DIFFERENTIAL CALCULUS ON THE SPACE OF COUNTABLE LABELLED GRAPHS

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ABSTRACT. The study of very large graphs is becoming increasingly prominent in modern-day mathematics. In this paper we develop a rigorous foundation for studying the space of finite labelled graphs and their limits. These limiting objects are naturally countable graphs, and the completed graph space $\mathcal{G}(V)$ is identified with the 2-adic integers as well as the Cantor set. The goal of this paper is to develop a model for differentiation on graph space in the spirit of the Newton-Leibnitz calculus. To this end, we first study the space of all finite labelled graphs and their limiting objects, and establish analogues of left-convergence, homomorphism densities, a Counting Lemma, and a large family of topologically equivalent metrics on labelled graph space. We then establish results akin to the First and Second Derivative Tests for real-valued functions on countable graphs, and completely classify the permutation automorphisms of graph space that preserve its topological and differential structures.

1. INTRODUCTION

Large amounts of modern data comes in the form of networks/graphs, as compared to standard discrete or continuous data that lives on the integers or the real line respectively. Thus, subjects like Erdős-Rényi random graphs, finite (large) graphs and their limits have a vast number of applications - to social networks (e.g., friendship graph), the internet (and world-wide web), ecological and biological networks (such as the human brain), resistance networks and chip design among others. In recent times, these areas have become the subject of a large body of literature. An important feature of these networks is that they are always changing (increasing) with respect to time. Additional vertices and edges are being added to the network, which makes the study of large graphs and their limits - in a unified setting - a necessary and important subject.

There are several significant strides that have been made in the literature. Prominent among them is the comprehensive, unifying theory developed by Borgs, Chayes, Lovász, Sós, Szegedy, Vesztegombi, and several others. In this (unlabelled) theory the space of *graphons* was introduced and studied; see e.g. [BCLSV, LS1] as well as the comprehensive monograph [Lo] (and the references therein) for more on graphons. These are symmetric measurable functions $: [0, 1]^2 \rightarrow [0, 1]$. It is shown that the space of weak equivalence classes of graphons is a compact path connected metric space, and the notion of graph limits (of “dense unlabelled graphs”) coincides with that of limits in this metric. There is a large body of work on related subjects such as random graphs, subgraph sampling, parameter testing, and other topics.

Some of the future challenges of applying the theory of graphons to real-world networks involve labelling and density issues. First, graphs in real-life network data are usually labelled, and one often needs to distinguish between vertices as each vertex has a specific meaning (for instance in a person-to-person network). A second reason is that in real-world situations the underlying graphs are often sparse. Hence results on limits of dense graph sequences may not be as applicable. There has been tremendous activity on extending results from dense graph limit theory to various sparse settings, including bounded degree graphs, sparse graphs without dense spots, locally rooted trees,

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graphings, and very recently, an L^p -theory of sparse graphs. See [BJR, BR, BCCZ1, BCCZ2, Lo], and the references therein.

In this paper, we focus on the first motivation: namely, to study finite labelled graphs and their limits. A necessary first step in studying such notions is to develop a suitable framework in which to study all finite labelled graphs at once. One way to proceed is to construct a space containing the countable set of all finite graphs, and then to study the topology of this space, as it pertains to the limits of finite graphs. Having done so, our next step is to develop a framework for studying functions on this space. For instance, it is of immense interest to be able to maximize real-valued functions on graphs. This requires developing a comprehensive theory of differential calculus on graphs. In particular, can a version of the First Derivative Test be formulated and proved for real-valued functions on graphs? At present, such a theory does not exist in the labelled setting. Hence a framework that allows the space of graphs to be treated as a continuum, armed with a graph calculus, could have tremendous benefits and was one of the main motivations of this paper.

The study of limits of finite labelled graphs is also interesting in that one encounters several parallel results to the development of the theory of graphons. For instance, the notion of left-convergence of a labelled graph sequence can be made precise in terms of “homomorphism indicators”. There exists a large family of topologically equivalent metrics which metrizes the topology of left-convergence. We also formulate analogues of the Counting Lemma, the Inverse Counting Lemma, and a Weak Regularity Lemma for labelled graphs. Moreover, we show a representation theorem wherein limits of left-convergent sequences of finite labelled graphs are graphs with countably many vertices. The space of graphs and their limits is shown to be a compact metric space.

At the same time there are several key differences between the labelled theory and the graphon setting. The fundamental difference is that one no longer quotients out by permutation automorphisms (or the group of measure-preserving bijections on $[0, 1]$) in the labelled setting. Thus, adding additional nodes (but no edges) changes the underlying graphon; but in our setting, for labelled graphs the underlying vertex set is already fixed - i.e., non-isolated nodes come with additional “ghost vertices” in the fixed vertex set. There are also other distinctions. For instance, countable labelled graphs form a compact and totally disconnected group, whereas the space of graphons is path-connected and has no natural group structure on it. Moreover, limits of sparse graphs in the dense theory are always zero (under the cut metric) while in the labelled setting we treat sparse and dense labelled graphs on an equal footing. The limit of a sparse graph sequence can even be an infinite graph. Finally, we add that in joint work [DGKR] with Diao and Guillot, we have initiated the study of differential calculus in the graphon setting as well; yet there are significant distinctions between that work and the present paper, owing to the two different topological structures.

Organization. We briefly outline the organization of the paper. In Section 2 we introduce the space of graphs $\mathcal{G}(V)$ on a countable labelled vertex set V , and develop initial results in topology and analysis for $\mathcal{G}(V)$. We also introduce and study homomorphism indicators, which parallel homomorphism densities in the graphon setting including through a Counting Lemma and left-convergence. We then develop a theory of Newton-Leibnitz differentiation on $\mathcal{G}(V)$ in Section 3, and prove various results including a version of the First Derivative Test. We also completely classify the effect of permutation automorphisms on the topological and differential structure of $\mathcal{G}(V)$. Finally, in Section 4 we initiate the study of an interesting summary statistic for countable graphs: the limiting edge density.

2. THE SPACE OF COUNTABLE LABELLED GRAPHS: TOPOLOGY AND HOMOMORPHISM INDICATORS

Consider an arbitrary vertex set V . Let $\mathcal{G}(V)$ denote the space of all labelled graphs with vertices in the (labelled) set V , and no self-loops or repeated edges between vertices (but possibly

isolated vertices). Let $\mathcal{G}_0(V)$ and $\mathcal{G}_1(V)$ denote the sets of graphs on V which have finitely many edges and co-finitely many edges respectively, and define $\mathcal{G}'(V) := \mathcal{G}(V) \setminus (\mathcal{G}_0(V) \cup \mathcal{G}_1(V))$. Also denote by K_V the complete graph on V . Throughout this paper, when the vertex set V is specified we will identify a graph $G = (V, E)$ with its set of edges $E \subset K_V$; thus, all graphs in $\mathcal{G}(V)$ are subsets of K_V . In other words, every graph with labelled vertex set V is associated with a function $G : K_V \rightarrow \{0, 1\}$, or equivalently, with a symmetric function $f^G : V \times V \rightarrow \{0, 1\}$ which is zero on the diagonal. Note that this is parallel to the unlabelled setting, in which every finite simple graph G is associated with a graphon, i.e., a symmetric step-function $f^G : [0, 1] \times [0, 1] \rightarrow [0, 1]$ which is zero on the diagonal.

Under some abuse of notation, we also write $\mathcal{G}(V) = \mathcal{P}(K_V) = (\mathbb{Z}/2\mathbb{Z})^{K_V}$, which is a commutative unital $\mathbb{Z}/2\mathbb{Z}$ -algebra. On the level of subsets of K_V , the pointwise addition and multiplication in $(\mathbb{Z}/2\mathbb{Z})^{K_V}$ correspond to taking the symmetric difference and intersection, respectively. In other words, if $G_i = (V, E_i)$ are graphs in $\mathcal{G}(V)$ for $i = 1, 2$, then the algebra operations are as follows:

$$G_1 \pm G_2 := (V, E_1 \Delta E_2), \quad G_1 \cdot G_2 := (V, E_1 \cap E_2), \quad \mathbf{1}_{\mathcal{G}(V)} := K_V, \quad \bar{0} \cdot G_1 := \mathbf{0}, \quad \bar{1} \cdot G_1 := G_1,$$

where $\mathbf{0} = 0_{\mathcal{G}(V)} := (V, \emptyset)$ is the disconnected/empty graph on V .

2.1. Graph convergence. We introduce the following notion of convergence on $\mathcal{G}(V)$.

Definition 2.1. A sequence of graphs $G_n \in \mathcal{G}(V)$ is said to *converge* to a graph $G \in \mathcal{G}(V)$ if for every edge $e \in K_V$, the indicator sequence $\mathbf{1}_{e \in G_n}$ converges to $\mathbf{1}_{e \in G}$.

Note that this notion of graph convergence induces precisely the product topology on $\mathcal{G}(V) = (\mathbb{Z}/2\mathbb{Z})^{K_V}$. Thus the following properties of graph convergence in $\mathcal{G}(V)$ are standard.

Lemma 2.2. Fix a labelled set V , and identify each $G \in \mathcal{G}(V)$ with its set of edges.

- (1) If a sequence G_n in $\mathcal{G}(V)$ is convergent, then the limit is unique.
- (2) If $G_n \subset G_{n+1}$ (or $G_n \supset G_{n+1}$) for all n , then $\lim_{n \rightarrow \infty} G_n = \bigcup_{n \in \mathbb{N}} G_n$ (respectively, $\bigcap_{n \in \mathbb{N}} G_n$).
- (3) If $G_n \rightarrow G$ and $G'_n \rightarrow G'$ in $\mathcal{G}(V)$ as $n \rightarrow \infty$, then $G_n + G'_n \rightarrow G + G'$ and $G_n \cdot G'_n \rightarrow G \cdot G'$. (Here, $+$:= Δ and \cdot := \cap , as above.)
- (4) G_n converges (to G) if and only if for all finite subsets $E_0 \subset K_V$, the sets $E_0 \cap G_n$ are eventually constant (and their limit equals $E_0 \cap G$).

Note that if G_n is an increasing sequence of graphs, then ordinary intuition suggests that the limit should be their union (i.e., the union of their edge sets); and similarly, the limit of a decreasing sequence should naturally be their common intersection. This is made precise by Lemma 2.2. In turn, the lemma helps summarize the topological properties of graph space $\mathcal{G}(V)$:

Proposition 2.3. For any set V , $\mathcal{G}(V)$ is a totally disconnected, compact, abelian, topological $\mathbb{Z}/2\mathbb{Z}$ -algebra. The notion of graph limits above, agrees with the same notion in this (Hausdorff) topology. The sets $\mathcal{G}_0(V)$ and $\mathcal{G}_1(V)$ are always dense in $\mathcal{G}(V)$ (so $\mathcal{G}(V)$ is separable if V is countable). Moreover, $\mathcal{G}(V)$ is perfect if and only if V is infinite.

Since $\mathcal{G}(V)$ is not connected, we remark that the Intermediate Value Theorem does not hold for $\mathcal{G}(V)$. For the same reason, the notion of convex functions does not make sense on $\mathcal{G}(V)$.

Proof. Note that $\mathcal{G}(V) = (\mathbb{Z}/2\mathbb{Z})^{K_V}$, and $\mathbb{Z}/2\mathbb{Z} = \{0, 1\}$ is a compact, discrete abelian group. By Lemma 2.2(3), the algebra operations are continuous with respect to the notion of convergence above; but this is precisely the same as coordinatewise convergence, so the operations are all continuous with respect to the product topology. Most of the remaining assertions are standard. Finally, we claim that (co)finite graphs are dense in $\mathcal{G}(V)$. To show the claim, use the standard

subbase of open sets for the product topology. Thus, given any open neighborhood U of a graph $G \in \mathcal{G}(V)$, there exist $n \in \mathbb{N}$ and edges $e_1, \dots, e_n \in K_V$ such that the open cylinder

$$\{G' \in \mathcal{G}(V) : \mathbf{1}_{e_i \in G'} = \mathbf{1}_{e_i \in G} \forall 1 \leq i \leq n\}$$

is contained in U . Now define

$$G_0 := G \cap \{e_1, \dots, e_n\}, \quad G_1 := G_0 \coprod (K_V \setminus \{e_1, \dots, e_n\}).$$

Then $G_i \in \mathcal{G}_i(V)$ for $i = 0, 1$. This shows that every open neighborhood U of any $G \in \mathcal{G}(V)$ contains at least one finite graph G_0 and co-finite graph G_1 . The claim immediately follows. \square

Remark 2.4. Note that the above notion of convergence resembles that of left-convergence for graphons. This is made more precise in Section 2.3 by introducing “homomorphism indicators”, which are analogues in the labelled setting of homomorphism densities. Homomorphism indicators turn out to be continuous on graph space and to satisfy a Stone-Weierstrass type result; additionally, they lead naturally to a notion of left-convergence in the labelled setting.

2.2. Metrics on graph space. Some natural questions that now arise are if the aforementioned topology on graph space $\mathcal{G}(V)$ is metrizable, or for which vertex sets V does every sequence of graphs possess a convergent subsequence. The following result answers these questions.

Proposition 2.5. *If V is countable, then every sequence $\{G_n : n \in \mathbb{N}\}$ in $\mathcal{G}(V)$ has a convergent subsequence (with the above definition). If V has cardinality at least that of the continuum, then this statement is false. In particular, the product topology here is not metrizable.*

If the product topology is metrizable when V is countable (as it is not when $|V| \geq |\mathbb{R}|$), then the first assertion above is a consequence of the fact that compactness is equivalent to sequential compactness. We show below that this is indeed the case.

Proof. If V is countable, then $\mathcal{G}(V)$ is a countable product of sequentially compact spaces $\mathbb{Z}/2\mathbb{Z} = \{0, 1\}$ and is thus sequentially compact. On the other hand, suppose $|V| \geq |\mathbb{R}|$; then V is infinite, so $|V| = |K_V|$. Moreover, by assumption there exists an injection $\pi : \mathcal{P}(\mathbb{N}) \hookrightarrow K_V$ from the set of all subsets of \mathbb{N} to the set of all edges in K_V , since $|\mathcal{P}(\mathbb{N})| = |\mathbb{R}| \leq |V| = |K_V|$. Now consider the sequence of graphs $G_n \in \mathcal{G}(V)$, where G_n consists of the edges

$$G_n = \{e_{\pi(I)} : I \subset \mathbb{N}, n \in I\} \subset K_V.$$

We claim that $\{G_n : n \in \mathbb{N}\}$ has no convergent subsequence. To show the claim, given $\{G_{n_k} : k \in \mathbb{N}\}$ with $n_1 < n_2 < \dots$, define $I := \{n_{2k} : k \in \mathbb{N}\}$. Then $\mathbf{1}_{e_{\pi(I)} \in G_{n_k}} = 0, 1, 0, 1, \dots$, which is not eventually constant.

Finally, if there exists a metric on $\mathcal{G}(V)$ when $|V| \geq |\mathbb{R}|$ such that the induced topology is the product topology, then $\mathcal{G}(V)$ would be compact, hence sequentially compact, which is false. \square

Henceforth we focus on the case when V is countable. In this case, we say that graphs $G \in \mathcal{G}(V)$ are *countable graphs*. Such graphs form the focus of the present paper because by Lemma 2.2, the set of countable graphs agrees exactly with the set of limits of sequences of finite graphs (i.e., graphs with finitely many edges).

Similar to the graphon case, we now discuss how to metrize graph convergence in $\mathcal{G}(V)$ for countable V .

Definition 2.6. Suppose V is countable. Define $\ell_+^1(K_V)$ to be the set of all maps $\varphi : K_V \rightarrow (0, \infty)$ such that $\sum_{e \in K_V} \varphi(e)$ is finite. Given $\varphi \in \ell_+^1(K_V)$, define $d_\varphi : \mathcal{G}(V) \times \mathcal{G}(V) \rightarrow \mathbb{R}$ via:

$$d_\varphi(G_1, G_2) = \sum_{e \in G_1 \Delta G_2} \varphi(e).$$

Recall [AKM] that when G_1, G_2 are finite, the *edit distance* or *Hamming distance* is defined to be the cardinality $|G_1 \Delta G_2|$. Since the graphs in the space of interest $\mathcal{G}(V)$ are countable, it is natural to work with weighted variants of the Hamming distance. This explains the decision to work with the functions in $\ell_1^+(K_V)$. Now the following result follows from standard arguments.

Proposition 2.7. *Suppose V is countable. Then for all $\varphi \in \ell_1^+(K_V)$ the maps d_φ are translation-invariant metrics which metrize the product topology on $\mathcal{G}(V)$.*

In particular, all metrics d_φ are topologically equivalent on $\mathcal{G}(V)$. Note also that in defining and studying the metrics d_φ , we do not use any ordering on the vertices or the edges of K_V , either explicitly or implicitly. This is because all of the metrics are topologically equivalent, so that the actual choice of labelling on the graphs in $\mathcal{G}(V)$ does not affect the underlying topology on $\mathcal{G}(V)$. In fact there is a larger family of metrics on graph space which are topologically equivalent; see Proposition 3.18 below.

Remark 2.8. We add for completeness that in the present paper we do not consider graphs with self-loops; however, our model of graph space $\mathcal{G}(V)$ can easily be amended to consider such graphs, by using the countable edge set of \overline{K}_V , the complete graph on V that also includes self-loops. Then all of the results in this paper also hold in the new model of graph space $\overline{\mathcal{G}}(V) = 2^{\overline{K}(V)}$ as well, since it is once again a compact metric group (isomorphic to $\mathcal{G}(V)$).

2.3. Homomorphism indicators. In the analysis of unlabelled graphs and their limits, homomorphism densities play a fundamental and important role. In particular, homomorphism densities provide a characterization of convergence of graph sequences called left convergence. We now introduce an analogous family of functions in the labelled setting and show how it can be used to characterize graph convergence. We also prove other results for this family, parallel to results for hom-densities in the graphon literature.

Definition 2.9. Given labelled graphs $H, G \in \mathcal{G}(V)$ on an arbitrary labelled vertex set V , define the *injective homomorphism indicator* $t'_{\text{inj}}(H, G)$ to be the indicator of the event that H occurs as a subgraph of G . Similarly define the *induced homomorphism indicator* $t'_{\text{ind}}(H, G)$ to be the indicator of the event that H occurs as an induced subgraph of G .

A sequence of countable graphs $G_n \in \mathcal{G}(V)$ is said to *left converge* (to a graph $G \in \mathcal{G}(V)$) if the corresponding sequences of injective homomorphism indicators $t'_{\text{inj}}(H, G_n)$ converges (to $t'_{\text{inj}}(H, G)$) for all finite graphs $H \in \mathcal{G}_0(V)$.

One can similarly define a notion of graph limits using the induced homomorphism indicators. It is now natural to ask if graph convergence can be encoded using either of these families of homomorphism indicators. The following result provides a positive answer to the question.

Lemma 2.10 (Inclusion-exclusion and left-convergence). *Given any labelled vertex set V and a finite graph $H \in \mathcal{G}_0(V)$, the induced and injective homomorphism indicators from H are related as follows:*

$$t'_{\text{inj}}(H, G) = \sum_{H \subset H' \subset K_{V(H)}} t'_{\text{ind}}(H', G), \quad t'_{\text{ind}}(H, G) = \sum_{H \subset H' \subset K_{V(H)}} (-1)^{|E(H' \setminus H)|} t'_{\text{inj}}(H', G), \quad (2.11)$$

for all $G \in \mathcal{G}(V)$. (Here $V(H)$ denotes the non-isolated nodes of H .) Moreover, the topologies induced by left-convergence and by the convergence of the induced homomorphism indicators, both coincide with the Hausdorff product topology on $\mathcal{G}(V)$.

Furthermore, for any left-convergent sequence of graphs on an arbitrary labelled vertex set V , there exists a (unique) limiting object in $\mathcal{G}(V)$.

Consequently, a sequence of countable graphs is left-convergent if and only if it is a Cauchy sequence in the d_φ metric for any $\varphi \in \ell_1^+(K_V)$.

Proof. We first show Equation (2.11). Define $H'_G := G \cap K_{V(H)}$ for $G \in \mathcal{G}(V)$. Then $t'_{\text{ind}}(H', G) = \delta_{H', H'_G}$ for all $H \subset H' \subset K_{V(H)}$. The first equality in Equation (2.11) now follows, and from it the second equality is deduced by Möbius inversion in the poset of subgraphs of $K_{V(H)}$.

In particular, it follows from Equation (2.11) that the topologies induced by the two families of homomorphism indicators coincide. Now if H is the graph with precisely one edge e , then $t'(e, G) = \mathbf{1}_{e \in G}$. More generally, for any finite graph $H \in \mathcal{G}_0(V)$,

$$t'_{\text{inj}}(H, G) = \prod_{e \in H} t'_{\text{inj}}(e, G) = \prod_{e \in H} \mathbf{1}_{e \in G}, \quad t'_{\text{ind}}(H, G) = \prod_{e \in H} \mathbf{1}_{e \in G} \prod_{e \in K_{V(H)} \setminus H} \mathbf{1}_{e \notin G}. \quad (2.12)$$

It follows that the topology of left convergence agrees with coordinate-wise convergence, i.e., with the product topology. To show the final assertion, define the limiting object to have $e \in K_V$ as an edge if and only if the indicator sequence $\mathbf{1}_{e \in G_n}$ is eventually 1. \square

We now prove certain fundamental properties of homomorphism indicators. We term the following result as the *Counting Lemma* for countable labelled graphs, given its similarity to the Counting Lemma for graphons [Lo], which says that homomorphism densities are Lipschitz functions with respect to the cut-norm.

Theorem 2.13 (Counting Lemma for labelled graphs). *Suppose V is any set, and $I_0, I_1 \subset K_V$ are disjoint. Let $f_{I_0, I_1} : \mathcal{G}(V) \rightarrow \{0, 1\}$ be the indicator of the event that the edges in I_0 are not in a graph, while the edges in I_1 are. Then the following are equivalent:*

- (1) f_{I_0, I_1} is locally constant.
- (2) f_{I_0, I_1} is continuous.
- (3) $I_0 \amalg I_1$ is finite.

If V is countable and $\varphi \in \ell_+^1(K_V)$ induces the translation-invariant metric d_φ on $\mathcal{G}(V)$, then the above conditions are also equivalent to:

- (4) $f_{I_0, I_1} : (\mathcal{G}(V), d_\varphi) \rightarrow \mathbb{R}$ is Lipschitz (for any φ).

In this case f_{I_0, I_1} has “best” possible Lipschitz constant equal to $1/\min_{e \in I_0 \amalg I_1} \varphi(e)$.

In particular, the Counting Lemma holds for all induced and injective homomorphism indicators.

Proof. That (3) \implies (1) follows by considering the product topology, and (1) \implies (2) because the cylinder open sets in the product topology of $\mathcal{G}(V)$ are also closed. We now assume that $I_0 \amalg I_1$ is infinite and show that (2) fails. Suppose I_1 is infinite (the proof is similar for I_0 infinite). Then I_1 contains a countable set $I'_1 : \{(v_{i_n}, v_{j_n}) : n \in \mathbb{N}\}$ for some vertices $v_{i_n} \neq v_{j_n}$. Define $G_n := (K_V \setminus (I_0 \amalg I'_1)) \amalg \{(v_{i_1}, v_{j_1}), \dots, (v_{i_n}, v_{j_n})\}$ for all n . Then it is clear that $G_n \rightarrow K_V \setminus I_0$. However, $f_{I_0, I_1}(G_n) = 0$ for all n while $f_{I_0, I_1}(K_V \setminus I_0) = 1$. Therefore f_{I_0, I_1} is not continuous at $K_V \setminus I_0$ and (2) fails to hold. This proves that (1)–(3) are equivalent for any labelled vertex set V .

Now suppose V is countable. Then clearly (4) \implies (2). Conversely suppose (3) holds, and $G, G' \in \mathcal{G}(V)$. Then $|f_{I_0, I_1}(G) - f_{I_0, I_1}(G')|$ is either 0 or 1, so to show that f_{I_0, I_1} is Lipschitz we only need to consider the pairs of graphs G, G' for which the above difference is 1. But this implies that at least one of the indicators $\{\mathbf{1}_{e \in H} : e \in I_0 \amalg I_1\}$ attains distinct values for $H = G, G'$. In particular, $G \Delta G'$ has nonempty intersection with the finite subset $I_0 \amalg I_1$ of K_V . Now set $c_I := \min_{e \in I} \varphi(e)$ for all $I \subset K_V$. Then $d_\varphi(G, G') \geq c_{I_0 \amalg I_1}$, whence

$$|f_{I_0, I_1}(G) - f_{I_0, I_1}(G')| = 1 \leq \frac{1}{c_{I_0 \amalg I_1}} d_\varphi(G, G').$$

The same inequality clearly holds if $|f_{I_0, I_1}(G) - f_{I_0, I_1}(G')| = 0$, which proves (4) as desired. Finally, that $1/c_{I_0 \amalg I_1}$ is the best possible Lipschitz constant follows by considering $G = \emptyset$ and $G' = \{e'\}$, where e' is any edge which minimizes φ over $I_0 \amalg I_1$. \square

Remark 2.14. Note that one can also formulate a variant of the Inverse Counting Lemma for countable labelled graphs; however, this is obvious for $\mathcal{G}(V)$. This variant states that if for two graphs $G_1, G_2 \in \mathcal{G}(V)$ the difference of the homomorphism indicators $|t'(e, G_1) - t'(e, G_2)|$ is smaller than 1 for all edges $e \in K_V$, then $G_1 = G_2$. One can use either induced or injective homomorphism indicators in this case, because they agree on all finite graphs which are complete.

We end this part with two further properties that are satisfied by the homomorphism indicators in the labelled setting (as also by the hom-densities in the unlabelled setting).

Proposition 2.15 (Stone-Weierstrass; Lagrange Interpolation). *Suppose V is any labelled vertex set. The linear span of homomorphism indicators of all finite graphs is dense in the space of continuous real-valued functions on $\mathcal{G}(V)$.*

Moreover, given graphs $G_1, \dots, G_k \in \mathcal{G}(V)$ and arbitrary real numbers a_1, \dots, a_k , there exists a finite set of finite graphs $H_1, \dots, H_m \in \mathcal{G}_0(V)$ and constants $c_i \in \mathbb{R}$ such that $\sum_{i=1}^m c_i t'(H_i, G_j) = a_j$ for all $1 \leq j \leq k$.

Note that both assertions involve the linear span of all homomorphism indicators of finite graphs $\{t'(H, -) : H \in \mathcal{G}_0(V)\}$; thus, the result holds for both the injective and induced homomorphism indicators, by Equation (2.11).

Proof. The first part follows from the usual Stone-Weierstrass Theorem since the homomorphism indicator of the “empty graph” is the constant function 1, and the aforementioned linear span is indeed a subalgebra that separates points (e.g., if $e \in G \Delta G'$ then $t'_{\text{ind}}(e, -) = t'_{\text{inj}}(e, -)$ separates G and G'). For the second part, it suffices to demonstrate the existence of such graphs H_i and constants c_i such that $a_1 = 1$ and $a_2 = \dots = a_k = 0$. To see why this holds, given any $1 < j$, choose an edge $e_j \in G_1 \Delta G_j$. Then

$$\prod_{j=2}^k (\mathbf{1}_{e_j \in G_1} t'(e_j, -) + \mathbf{1}_{e_j \in G_j} (1 - t'(e_j, -)))$$

satisfies the given requirements. \square

3. DIFFERENTIAL CALCULUS ON COUNTABLE GRAPHS

We now come to the main goal of this paper: to establish a theory of differential calculus on graph space $\mathcal{G}(V)$, and to prove results in Newton-Leibnitz calculus such as an analogue of the First Derivative Test, on $\mathcal{G}(V)$. We remark that a theory of differential calculus on graphon space was recently established in a parallel paper [DGKR] for unlabelled graphs. Developing a calculus on labelled graph space $\mathcal{G}(V)$ also naturally follows in the progression of results developed, from topology, to analysis of graph space, to a deeper study of functions defined on $\mathcal{G}(V)$. In particular, akin to an application of differential calculus on the real line, one would like to ask: given a “score function” on graph space, is it possible to maximize or minimize it? We now propose a mechanism to answer this question using a formalism akin to the usual Newton-Leibnitz theory on \mathbb{R} .

3.1. A special family of metrics on graph space. The goal of this subsection is to identify a large subset of graph space with a more familiar topological model. To this end, we introduce and study a special family $\|\cdot\|_{\psi, a}$ of metrics on countable graph space $\mathcal{G}(V)$. This family of metrics is important for several reasons: (i) it helps find a more familiar model for $\mathcal{G}(V)$, (ii) it plays a crucial role in the theory of differential calculus developed in the present paper, and (iii) it will also be crucially used in a subsequent paper [KR] in developing integration and probability theory on $\mathcal{G}(V)$.

Definition 3.1. Given a countable labelled vertex set V and a bijection $\psi : K_V \rightarrow \mathbb{N}$, $a > 1$, and a graph $G = (V, E)$, define

$$\|G\|_{\psi,a} := \sum_{e \in E} a^{-\psi(e)}, \quad E_n(\psi) := \{e \in K_V : \psi(e) \leq n\}.$$

Also denote by \mathbb{D}_2 the set of dyadic rationals, i.e., rational numbers with a finite binary expansion.

Note that $\|\cdot\|_{\psi,a}$ is precisely the map $d_{\varphi_a}(\mathbf{0}, -)$, where $\varphi_a \in \ell_+^1(K_V)$ is defined via: $\varphi_a(G) := \sum_{e \in G} a^{-\psi(e)}$. Thus it too metrizes the product topology on $\mathcal{G}(V)$, for all $a > 1$.

We now study basic properties of the family $\|\cdot\|_{\psi,a}$ of metrics on graph space. The first observation is that the metric $\|\cdot\|_{\psi,a}$ satisfies an analogue of the Weak Regularity Lemma. More precisely, a countable graph can be “ ϵ -approximated” by a finite graph with $O(\log \epsilon^{-1})$ edges. The proof is straightforward and hence omitted.

Lemma 3.2 (Weak Regularity Lemma for labelled graphs). *Fix $a > 1$ and $\epsilon > 0$. Given $G \in \mathcal{G}(V)$, there exists a graph $G_0 \in \mathcal{G}_0(V)$ with at most $1 + \log(\epsilon(a-1))/\log(a)$ edges, such that $\|G - G_0\|_{\psi,a} < \epsilon$.*

This result is akin to the well-known Weak Regularity Lemma for unlabelled graphs shown by Frieze and Kannan [FK], where one needs a graph with $\sim 2^{40\epsilon^{-2}}$ edges to approximate a weighted graph with $\sim \epsilon^{-1}$ edges. In the labelled setting, the edges in G_0 can be chosen independently of $G \in \mathcal{G}(V)$. Note that given G or $\|G\|_{\psi,2}$, it is easy to approximate G as closely as desired: truncating the binary expansion of G at, say, the N th place yields precisely $G \cap E_N(\psi)$. Moreover, observing only the edges - or interactions - between “previously identified key nodes” is a linear time process, and one which reduces to computations in finite graph theory.

We now state some further properties of the family of metrics $\|\cdot\|_{\psi,a}$ for $a > 1$. For example, the uniqueness (outside a countable set) of writing a number in binary notation implies a similar property for $\|\cdot\|_{\psi,2} : \mathcal{G}(V) \rightarrow [0, 1]$.

Proposition 3.3. *Suppose $\psi : K_V \rightarrow \mathbb{N}$ is an injection.*

- (1) *If $\|\cdot\|_{\psi,a} : \mathcal{G}(V) \rightarrow [0, \|K_V\|_{\psi,a}]$ is surjective, then $1 < a \leq 2$. The converse holds if ψ is a bijection.*
- (2) *If $a > 2$, then $\|\cdot\|_{\psi,a}$ is injective on $\mathcal{G}(V)$. The converse holds if ψ is a bijection. More precisely, if $a \leq 2$, ψ is a bijection, and $G \in \mathcal{G}_0(V)$ is finite and nonempty, then there exists $G' \neq G$ such that $\|G\|_{\psi,a} = \|G'\|_{\psi,a}$.*
- (3) *Suppose ψ is a bijection and $a = 2$. Then $\|\cdot\|_{\psi,2} : \mathcal{G}(V) \rightarrow [0, 1]$ is a surjection such that every preimage has size at most two. More precisely, for all finite nonempty graphs G such that $\psi(G) = \{n_1 < \dots < n_k\} \subset \mathbb{N}$,*

$$\|G\|_{\psi,2} = \left\| \psi^{-1} \left(\{n_1, \dots, n_{k-1}\} \coprod \{n_k + 1, n_k + 2, \dots\} \right) \right\|_{\psi,2},$$

and $\|\cdot\|_{\psi,2}$ is a bijection onto $[0, 1]$ outside finite graphs - i.e., on $\mathcal{G}(V) \setminus \mathcal{G}_0(V)$ - as well as outside co-finite graphs.

- (4) *If $a \geq 2$ and ψ is a bijection, then the map $\|\cdot\|_{\psi,a} : K_V \rightarrow [0, 1]$ is order-preserving with respect to the lexicographic order on K_V (arranged according to $\psi^{-1}(1), \psi^{-1}(2), \dots$).*

Remark 3.4. If $a \in (2, \infty)$ then the $\|\cdot\|_{\psi,a}$ -weak norm is injective but not surjective, while at $a = 2$, it is injective except on the countable set of finite and co-finite graphs. If $a \in (1, 2)$ then $\|\cdot\|_{\psi,a}$ is surjective from $\mathcal{G}(V)$ onto an interval, but not injective. How “non-injective” does $\|\cdot\|_{\psi,a}$ get in this case? The following result asserts that for all but countably many algebraic numbers a , the answer is: on an uncountable set. As the result is not relevant to the main focus of the paper, its proof is omitted.

Proposition 3.5. *Suppose $\phi := (1 + \sqrt{5})/2$ is the golden ratio, and either $a \in (1, \phi]$, or $a \in (\phi, 2)$ is transcendental. Also assume that $\psi : K_V \rightarrow \mathbb{N}$ is a bijection, and $G \in \mathcal{G}_0(V)$ is finite. Then there exist uncountably many graphs $G' \supset G$ such that $\|G'\|_{\psi,a} = \|G''\|_{\psi,a}$ for some $G'' \neq G'$ also containing G .*

Proposition 3.5 is also related to *interval-filling sequences*; see [DJK1, DJK2] for more on these. Moreover, the phase transition occurring at 2, as discussed in Remark 3.4, is crucially used later in this section.

It is now possible to state and prove the main result of this subsection. The result asserts that the maps $\|\cdot\|_{\psi,a}$ help identify more familiar models for graph space $\mathcal{G}(V)$.

Proposition 3.6. *Fix a countable set V and a bijection $\psi : K_V \rightarrow \mathbb{N}$. Define $\mathcal{G}'(V) \subset \mathcal{G}(V)$ to be the subset of countable graphs on V , which are neither finite nor cofinite. Then for each $a > 2$, the map $\|\cdot\|_{\psi,a}$ is a homeomorphism from $\mathcal{G}(V)$ onto its image in \mathbb{R} (which is the Cantor set for $a = 3$). The same holds for $a = 2$, when restricted to the dense subset $\mathcal{G}'(V)$ but not to any domain strictly containing $\mathcal{G}'(V)$.*

Proof. First suppose $a > 2$. By the closed map lemma, the bijection $\|\cdot\|_{\psi,a} : \mathcal{G}(V) \rightarrow \mathbb{R}$ is continuous and closed, hence a homeomorphism. That the image is the Cantor set for $a = 3$ is also easily shown, e.g. by results in [Cam].

Now suppose $a = 2$. (Note that the closed map lemma does not apply to $\mathcal{G}(V)$ since $\|\cdot\|_{\psi,2}$ is not a bijection on $\mathcal{G}(V)$.) Then $\|\cdot\|_{\psi,2} : \mathcal{G}'(V) \rightarrow [0, 1]$ is continuous and a bijection. We now show that $(\|\cdot\|_{\psi,2})^{-1} : [0, 1] \setminus \mathbb{D}_2 \rightarrow \mathcal{G}'(V)$ is also continuous. Suppose $\|G_n\|_{\psi,2} \rightarrow \|G\|_{\psi,2}$ in $[0, 1] \setminus \mathbb{D}_2$. In other words the “binary expansions” of G_n converge to that of G . But then for all k , the k th digit of the binary expansion - which corresponds to $\mathbf{1}_{\psi^{-1}(k) \in G_n}$ is eventually equal to the k th digit of G , since $\|\cdot\|_{\psi,2}$ is a bijection on $\mathcal{G}'(V)$. This shows that $G_n \rightarrow G$ in the product topology (in $\mathcal{G}'(V)$).

Finally, to show that $\mathcal{G}'(V)$ is maximal for the property of $\|\cdot\|_{\psi,2}$ being a homeomorphism, suppose $G \in \mathcal{G}_0(V)$. We will construct a sequence of graphs $G_n \in \mathcal{G}'(V)$ such that $\|G_n\|_{\psi,2} \rightarrow \|G\|_{\psi,2}$ but $G_n \not\rightarrow G$. Indeed, fix any partition of $\mathbb{N} \setminus \{1, \dots, \max(\psi(G))\}$ into two infinite subsets $S = \{m_n : n \in \mathbb{N}\}$ and T , and define

$$G_n := \psi^{-1}(T) \coprod \{\psi^{-1}(m_1), \dots, \psi^{-1}(m_n)\} \coprod G \setminus \{\psi^{-1}(\max(\psi(G)))\}.$$

Then $G_n \in \mathcal{G}'(V)$ satisfies the desired assertions, showing that $\|\cdot\|_{\psi,2}$ is not a homeomorphism on any set containing $\mathcal{G}'(V) \cup \{G\}$, for any finite graph $G \in \mathcal{G}_0(V)$. The proof is similar for $G \in \mathcal{G}_1(V)$. \square

3.2. Newton-Leibnitz differential calculus on graph space. We now provide a novel approach to developing differential calculus on labelled graph space. To do so, we propose a model that allows us to transport differentiation on \mathbb{R} to $\mathcal{G}(V)$. Using Proposition 3.6 (in a manner explained below), we first define the derivative on graph space $\mathcal{G}(V)$.

Definition 3.7 (Derivative of a function at a graph). Suppose V is countable, with fixed bijection $\psi : K_V \rightarrow \mathbb{N}$. Now given $f : \mathcal{G}(V) \rightarrow \mathbb{R}$, define its derivative at a graph $G \neq \mathbf{0}, K_V$ to be:

$$f'(G) := \lim_{G_1 \rightarrow G, G_1 \in \mathcal{G}'(V)} \frac{f(G_1) - f(G)}{\|G_1\|_{\psi,2} - \|G\|_{\psi,2}},$$

if this limit exists.

Remark 3.8. This version of the derivative is a natural candidate to work with, as it transports the topological structure of $[0, 1]$ into graph space. There is a further parallel to the usual derivative in one-variable calculus:

$$f'(x) = \lim_{y \rightarrow x} \frac{f(y) - f(x)}{y - x}.$$

Observe that if $y > x$ or $y < x$, then the denominator in the right-hand limit is positive or negative respectively. When defining the derivative $f'(G)$ above, the same holds for $G_1 \neq G$ in the lexicographic order on $\mathcal{G}(V)$, by using Proposition 3.3(4). We remark also that $f'(G)$ also equals the limit

$$\lim_{G_1 \rightarrow G, G_1 \in \mathcal{G}'(V)} \frac{f(G_1) - f(G)}{\|G_1 \setminus G\|_{\psi,2} - \|G \setminus G_1\|_{\psi,2}}.$$

We are now able to state and prove a version of the First and Second Derivative Tests on labelled graph space.

Theorem 3.9 (First and Second Derivative Tests). *Suppose $f : \mathcal{G}(V) \rightarrow \mathbb{R}$ is locally maximized at $G_0 \in \mathcal{G}(V)$, with $G_0 \neq \mathbf{0}, K_V$. Then G_0 is a critical point of f - i.e., $f'(G_0)$ is zero if it exists.*

Suppose instead that f is twice differentiable at a critical point $G_0 \neq \mathbf{0}, K_V$, and also continuous in a neighborhood of G_0 . If $f''(G_0) < 0$, then G_0 is a local maximum for f .

Proof. Given $\mathbb{U} \subset \mathbb{R}$ and $g : \mathbb{U} \rightarrow \mathbb{R}$, define the \mathbb{U} -derivative of g at $x_0 \in \overline{\mathbb{U}}$ to be

$$D^{\mathbb{U}}g(x_0) := \lim_{x \in \mathbb{U}, x \rightarrow x_0} \frac{g(x) - g(x_0)}{x - x_0},$$

if this (two-sided) limit exists. This definition is weaker than the usual notion of the derivative, which is the special case $\mathbb{U} = \mathbb{R}$. However, it also satisfies the standard properties of differentiation (for real-valued functions), such as the product, quotient, and chain rules. In particular, if x_0 is a local maximum and an interior point of $\overline{\mathbb{U}}$, then we can adopt the proof of the usual First Derivative Test to taking limits as $x \rightarrow x_0$, $x \in \mathbb{U}$. We conclude that $D^{\mathbb{U}}g(x_0) = 0$ at local extreme points x_0 which are interior points of $\overline{\mathbb{U}}$.

Now fix $\mathbb{U} := [0, 1] \setminus \mathbb{D}_2$, and suppose $f'(G_0)$ exists. Then observe that f is continuous at G_0 . Let $x_0 := \|G_0\|_{\psi,2}$, and consider the function $g : ([0, 1] \setminus \mathbb{D}_2) \cup \{x_0\} \rightarrow \mathbb{R}$, given by $g(x) := f(G_0)$ if $x = x_0$, and $f((\|\cdot\|_{\psi,2})^{-1}(x))$ otherwise. If G_0 is either finite or co-finite, then restrict to a sufficiently small neighborhood of G_0 ; this shows that if $G_1 \rightarrow G_0$ with $G_1 \in \mathcal{G}'(V)$, then $g(\|G_1\|_{\psi,2}) \rightarrow g(x_0)$. Now since $f'(G_0)$ exists, so does $D^{\mathbb{U}}g(x_0)$ by Proposition 3.6. Moreover, $f'(G_0) = D^{\mathbb{U}}g(x_0) = 0$ by the above analysis, since G_0 is a local maximum for f .

This proves the First Derivative Test; we now show the Second Derivative Test. Suppose $G_0 \neq \mathbf{0}, K_V$ is a critical point and $f''(G_0) < 0$. As above, this implies that $D^{\mathbb{U}}D^{\mathbb{U}}g(x_0) < 0$. Now adopt the proof of the Second Derivative Test to taking limits as $x \rightarrow x_0$, $x \in \mathbb{U} = [0, 1] \setminus \mathbb{D}_2$. Thus x_0 is a local maximum for g on $([0, 1] \setminus \mathbb{D}_2) \cup \{x_0\}$, whence G_0 is a local maximum for f on $\mathcal{G}'(V) \cup \{G_0\}$. We are now done since f is continuous near G_0 . \square

It is also not hard to show that the derivative in graph space satisfies the usual product, quotient, and chain rules. We write down two of these results; the proofs are as in one-variable calculus.

Lemma 3.10 (Product and Chain Rules). *Suppose $f, g : \mathcal{G}(V) \rightarrow \mathbb{R}$ are differentiable at $G \neq \mathbf{0}, K_V$, and $h : \mathbb{R} \rightarrow \mathbb{R}$ is differentiable at $f(G)$. Then $f \cdot g$ and $h \circ f$ are differentiable at G , and moreover,*

$$(f \cdot g)'(G) = f(G)g'(G) + f'(G)g(G), \quad (h \circ f)'(G) = h'(f(G))f'(G).$$

We have thus seen that the derivative in graph space satisfies several well-known properties in the one-variable theory on \mathbb{R} . We now show that it does not always satisfy a “translation-invariance” property.

Proposition 3.11. *Suppose $f : \mathcal{G}(V) \rightarrow \mathbb{R}$ is differentiable at $G \neq \mathbf{0}, K_V$. For each $G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, the function $g(G) := f(G + G_0)$ is differentiable at $G - G_0$, and $g'(G - G_0) = \pm f'(G)$. However, $g'(G - G_0)$ does not exist if $G_0 \in \mathcal{G}'(V)$ and $f'(G) \neq 0$.*

Proof. If $G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$ then it is not hard to see that for all $G \in \mathcal{G}(V)$ and G_1 sufficiently close to G , $\|G_1 + G_0\|_{\psi,2} - \|G + G_0\|_{\psi,2} = \pm(\|G_1\|_{\psi,2} - \|G\|_{\psi,2})$, with the choice of sign equal to $+$ or $-$ depending on if $G_0 \in \mathcal{G}_0(V)$ or $\mathcal{G}_1(V)$. It follows that $g'(G - G_0) = g'(G_0 - G) = \pm f'(G)$. (This is akin to saying that if $g(x) = f(1 \pm x)$ for $x \in \mathbb{R}$, then $g'(0) = \pm f'(1)$.)

Now suppose $G_0 \in \mathcal{G}'(V)$. Fix $G \in \mathcal{G}(V)$ and partition K_V into four components:

$$A_1 := G \setminus G_0, \quad A_2 := G \cap G_0, \quad A_3 := G_0 \setminus G, \quad A_4 := K_V \setminus (G \cup G_0).$$

We now define a graph $G' \in \mathcal{G}(V)$ to be *admissible (with respect to G, G_0)* if whenever A_j is infinite for $1 \leq j \leq 4$, the sets $G' \cap A_j$ and $A_j \setminus G'$ are also infinite. Then the following properties of admissible graphs are not hard to show: (a) such graphs always exist; (b) if a graph G' is admissible then so is $G' \cap \psi^{-1}([n, \infty))$ for all $n \in \mathbb{N}$; and (c) if G' is admissible then $G', G + G', G - G_0 + G' \in \mathcal{G}'(V)$. The last property can be shown by considering the cases when G is infinite or $K_V \setminus G$ is infinite, and similarly for $G - G_0$.

Now given a graph $G' \in \mathcal{G}(V)$, define $x_j(G') := \|G' \cap A_j\|_{\psi,2}$ for $1 \leq j \leq 4$. Then,

$$\frac{\|G + G'\|_{\psi,2} - \|G\|_{\psi,2}}{\|G - G_0 + G'\|_{\psi,2} - \|G - G_0\|_{\psi,2}} = \frac{x_3(G') + x_4(G') - x_1(G') - x_2(G')}{x_2(G') + x_4(G') - x_1(G') - x_3(G')}, \quad \forall G' \in \mathcal{G}(V). \quad (3.12)$$

Denote by $T(G')$ the quantity in Equation (3.12). Also note that $A_2 \cup A_3 = G_0$ and $A_1 \cup A_4 = K_V \setminus G_0$ are both infinite sets of edges since $G_0 \in \mathcal{G}'(V)$. Thus we can choose a sequence $G_n \in \mathcal{G}'(V)$ of graphs satisfying: (i) G_n is admissible with respect to G, G_0 ; (ii) $G_n \subset G_0 \cap \psi^{-1}([n, \infty))$; and (iii) $x_2(G_n) \neq x_3(G_n)$ for all n . For this sequence, we obtain $T(G_n) = -1$ for all n in Equation (3.12), whence using the hypothesis that $f'(G) \neq 0$, and the properties of admissibility, we compute:

$$\lim_{n \rightarrow \infty} \frac{g(G - G_0 + G_n) - g(G - G_0)}{\|G - G_0 + G_n\|_{\psi,2} - \|G - G_0\|_{\psi,2}} \cdot \left(\frac{f(G + G_n) - f(G)}{\|G + G_n\|_{\psi,2} - \|G\|_{\psi,2}} \right)^{-1} = \lim_{n \rightarrow \infty} T(G_n) = -1.$$

Thus we must have $g'(G - G_0) = -f'(G)$ if the left-hand side exists. Similarly, choose a sequence $G_n \in \mathcal{G}'(V)$ of graphs satisfying: (i) G_n is admissible with respect to G, G_0 ; (ii) $G_n \subset (K_V \setminus G_0) \cap \psi^{-1}([n, \infty))$; and (iii) $x_1(G_n) \neq x_4(G_n)$ for all n . For this sequence, we obtain $T(G_n) = 1$ for all n in Equation (3.12), whence $g'(G - G_0)$ must equal $f'(G)$ if it exists. We conclude that $g'(G - G_0)$ does not exist. \square

Remark 3.13. We also note for completeness that a different candidate for the definition of the derivative could also be explored, namely:

$$(D'f)(G) := \lim_{G_1 \rightarrow G, G_1 \in \mathcal{G}'(V)} \frac{f(G_1) - f(G)}{\|G_1 - G\|_{\psi,2}}.$$

Indeed, this formula is a special case of the notion of a derivative in an arbitrary metric space. This candidate for the derivative suffers from the drawback that if $(D'f)(G)$ exists for $G \in \mathcal{G}'(V)$, then by considering sequences of graphs $G_n \uparrow G$ and $G'_n \downarrow G$ in $\mathcal{G}'(V)$, it necessarily follows that $(D'f)(G) = 0$. For this reason we do not work with $D'f$ in the present paper.

3.3. Examples. We now discuss examples of functions on graph space which are differentiable (together with their derivatives). Our first family of examples comes from the ℓ_+^1 -family of metrics described above.

Proposition 3.14. *Suppose V is countable, $\psi : K_V \rightarrow \mathbb{N}$ is a fixed bijection, $G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, and $\varphi \in \ell_+^1(K_V)$. Define $f(G) := d_\varphi(G_0, G)$. Then the following are equivalent:*

- (1) $c_\varphi := \lim_{n \rightarrow \infty} 2^n \varphi(\psi^{-1}(n))$ exists.
- (2) $f'(G)$ exists for some G such that $G \Delta G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$.

In this case, $f'(G)$ exists whenever $G\Delta G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, in which case

$$f'(G) = \begin{cases} c_\varphi, & \text{if } G, G\Delta G_0 \in \mathcal{G}_0(V) \text{ or } G, G\Delta G_0 \in \mathcal{G}_1(V), \\ -c_\varphi, & \text{if } (G, G\Delta G_0) \in \mathcal{G}_i(V) \times \mathcal{G}_{1-i}(V) \text{ for some } i = 0, 1. \end{cases} \quad (3.15)$$

However, $f'(G)$ need not exist (or be nonzero if it exists), if $G \in \mathcal{G}'(V)$.

The result can be thought of as akin to computing the derivative of the metric function $f(x) = |x - a| : \mathbb{R} \rightarrow \mathbb{R}$ for any $a \in \mathbb{R}$. Note in the above result that both $d_\varphi(-)$ and $d_{\varphi_2}(\mathbf{0}, -) = \|\cdot\|_{\psi,2}$ are nondecreasing functions in the lexicographic order on $\mathcal{G}(V)$ (as in Proposition 3.3(4)).

Proof. We mention at the outset of this proof that since $G\Delta G_0, G_0$ (and hence G) all lie in $\mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, to compute derivatives in this proof it is equivalent to take limits as either $G_1 \rightarrow \mathbf{0}$, or as $G_1 \rightarrow G$ or $G_1 \rightarrow G\Delta G_0$ (with $G_1 \in \mathcal{G}'(V)$). Now suppose c_φ exists, and $G \in \mathcal{G}(V)$ is such that $G\Delta G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$. We show that Equation (3.15) holds; in particular, this shows that (1) \implies (2). Given a graph $G' \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, define $n_{G'} := \max \psi^{-1}(G')$ if $G' \in \mathcal{G}_0(V)$, and $\max \psi^{-1}(K_V \setminus G')$ if $G' \in \mathcal{G}_1(V)$. Note that $c_\varphi \geq 0$. Now given $\epsilon > 0$, choose an integer $N \gg 0$ such that $N > \max(n_{G\Delta G_0}, n_G)$ (since $G \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$) and $2^n \varphi(\psi^{-1}(n)) \in [\max(0, c_\varphi - \epsilon), c_\varphi + \epsilon]$ for all $n > N$. Now compute the derivative $f'(G)$ by considering $G_1 \rightarrow \mathbf{0}$ with $G_1 \in \mathcal{G}'(V)$ and $\|G_1\|_{\psi,2} < 2^{-N}$. By choice of N , it follows in both of the aforementioned cases that

$$\frac{f(G + G_1) - f(G)}{\|G + G_1\|_{\psi,2} - \|G\|_{\psi,2}} = \frac{d_\varphi(G\Delta G_0, G_1) - d_\varphi(G\Delta G_0, \mathbf{0})}{\|G\Delta G_1\|_{\psi,2} - \|G\|_{\psi,2}} = \pm \frac{\sum_{e \in G_1} \varphi(e)}{\sum_{e \in G_1} 2^{-\psi(e)}},$$

where the choice of signs is as specified in Equation (3.15). Note that the ratio of the two sums (without the signs) lies in $[\max(0, c_\varphi - \epsilon), c_\varphi + \epsilon]$ since $\|G_1\|_{\psi,2} < 2^{-N}$. This proves the assertion if $G\Delta G_0$ is finite or cofinite.

We next show that (2) \implies (1). Suppose $f'(G)$ exists with $G\Delta G_0$ finite or cofinite. Let $N := \max(n_{G\Delta G_0}, n_G)$ and consider $G_n := \psi^{-1}(N + n + 2\mathbb{N}) \in \mathcal{G}'(V)$. Then,

$$\frac{f(G + G_n) - f(G)}{\|G + G_n\|_{\psi,2} - \|G\|_{\psi,2}} = \frac{d_\varphi(G\Delta G_0, G_n) - d_\varphi(G\Delta G_0, \mathbf{0})}{\|G\Delta G_n\|_{\psi,2} - \|G\|_{\psi,2}} = \pm \frac{\sum_{k \in \mathbb{N}} \varphi(\psi^{-1}(N + n - 1 + 2k))}{\sum_{k \in \mathbb{N}} 2^{-(N+n-1+2k)}},$$

with the sign as in Equation (3.15) remaining unchanged for all n . Call the previous ratio (without the signs) a_n , and consider the odd and even terms of the convergent sequence $\{a_n : n \in \mathbb{N}\}$ separately. Each of these subsequences are ratios of tail sums of convergent series $\sum_{k \geq m} b_k$ and $c \sum_{k \geq m} 4^{-k}$, say. Now the subsequence converges, whence

$$\left| \frac{\sum_{k \geq m} b_k}{c \sum_{k \geq m} 4^{-k}} - \frac{\sum_{k \geq m+1} b_k}{c \sum_{k \geq m+1} 4^{-(k+1)}} \right| \rightarrow 0$$

as $m \rightarrow \infty$. Taking common denominators, we obtain:

$$\frac{4^{-m}}{\sum_{k \geq m} 4^{-k}} \cdot \left| \frac{b_m}{c 4^{-m}} - \frac{\sum_{k \geq m+1} b_k}{c \sum_{k \geq m+1} 4^{-k}} \right| = \frac{3}{4} \left| \frac{b_m}{c 4^{-m}} - \frac{\sum_{k \geq m+1} b_k}{c \sum_{k \geq m+1} 4^{-k}} \right| \rightarrow 0.$$

It follows that $b_m/(c 4^{-m}) \rightarrow \lim_n a_n$ as $m \rightarrow \infty$. In particular, the sequences $2^{N+2k} \varphi(\psi^{-1}(N+2k))$ and $2^{N-1+2k} \varphi(\psi^{-1}(N-1+2k))$ both converge, and to the common limit $\lim_{n \rightarrow \infty} a_n$. Hence $\lim_{n \rightarrow \infty} a_n = \lim_{n \rightarrow \infty} 2^n \varphi(\psi^{-1}(n)) = c_\varphi$ exists.

Finally, we study if $f'(G)$ exists and equals $\pm c_\varphi$ for all $G \in \mathcal{G}(V)$. Note that this indeed happens on occasion - for instance, if the function $\varphi(-)$ is a scalar multiple of $\|\cdot\|_{\psi,2}$ on K_V , and $G_0 \in \mathcal{G}_0(V) \cup \mathcal{G}_1(V)$, then clearly $f'(G) = \pm c_\varphi \forall G \in \mathcal{G}(V)$. However, we now show that if $G\Delta G_0 \in \mathcal{G}'(V)$, then $f'(G)$ may not exist or equal $\pm c_\varphi$ for general φ . Specifically, take $G_0 := \mathbf{0}$ and $G := \psi^{-1}(\mathbb{N} \setminus$

$(-3 + 4\mathbb{N})) \subset K_V$, so that $G\Delta G_0 \in \mathcal{G}'(V)$. Define $G_n := \{\psi^{-1}(2), \psi^{-1}(4), \dots, \psi^{-1}(4n); \psi^{-1}(4n-3)\} \cup (-1 + 4\mathbb{N})$, and $\varphi_2, \varphi_3 \in \ell_+^1(K_V)$ via:

$$\varphi_j(\psi^{-1}(4n-3)) := (1 - (4n-3)^{-j}) \cdot 2^{-4n}/3, \quad j = 2, 3,$$

and $\varphi_2(\psi^{-1}(m)) = \varphi_3(\psi^{-1}(m)) := 2^{-m}$ for all other $m \in \mathbb{N}$. Therefore $c_{\varphi_j} = 1$ for $j = 2, 3$; moreover, $G_n \in \mathcal{G}'(V)$ converges to G . Now set $f_j(G) := d_{\varphi_j}(G, \mathbf{0})$. If $f'_j(G)$ exists and is nonzero for $j = 2, 3$, then we compute:

$$0 \neq \frac{f'_3(G)}{f'_2(G)} = \lim_{n \rightarrow \infty} \frac{d_{\varphi_3}(G_n, \mathbf{0}) - d_{\varphi_3}(G, \mathbf{0})}{d_{\varphi_2}(G_n, \mathbf{0}) - d_{\varphi_2}(G, \mathbf{0})} = \lim_{n \rightarrow \infty} \frac{(1 - (4n-3)^{-3})(2^{-4n}/3) - 2^{-2-4n} \cdot (4/3)}{(1 - (4n-3)^{-2})(2^{-4n}/3) - 2^{-2-4n} \cdot (4/3)} = 0,$$

which is impossible. It follows that at least one of $f_{\varphi_2}, f_{\varphi_3}$ is not differentiable at $G \in \mathcal{G}'(V)$ with nonzero derivative, even though $c_{\varphi_2} = c_{\varphi_3} = 1$. \square

Note that more examples can be generated from differentiable functions by using the standard rules of differentiation (which also hold for graph space, as discussed in Lemma 3.10). We now discuss a third example, which can be obtained by adapting the p -adic norm to $\mathcal{G}(V)$. The proof of the following result is omitted for brevity.

Corollary 3.16. *If $f : \mathcal{G}'(V) \rightarrow \mathbb{R}$ is locally constant, then f is differentiable on $\mathcal{G}'(V)$, and $f' \equiv 0$ on $\mathcal{G}'(V)$. For instance, fix a function $\zeta : K_V \rightarrow (0, \infty)$ such that $\zeta(\psi^{-1}(n)) \rightarrow 0$ as $n \rightarrow \infty$ and $\zeta(K_V)$ has no other accumulation points. Now define $\|G\|_\zeta^\infty := \min_{e \in G} \zeta(e)$ and $\|\mathbf{0}\|_\zeta^\infty := 0$. Then $\|\cdot\|_\zeta^\infty$ is locally constant and hence has derivative zero.*

For example, one can choose $\zeta_p(\psi^{-1}(n)) := p^{-n}$ to be the “ p -adic norm” for $p > 1$. The function ζ_3 was used in [Cam] to identify graph space $\mathcal{G}(V)$ with the Cantor set. Also note that homomorphism indicators from finite graphs - and more generally the functions f_{I_0, I_1} studied in Theorem 2.13 - are locally constant, hence have zero derivative by Corollary 3.16.

Remark 3.17. The functions $\|\cdot\|_\zeta^\infty$ are of independent interest, being not only locally constant but also translation-invariant metrics on labelled graph space. More precisely, define $\ell_+^\infty(K_V)$ to be the set of all $\zeta : K_V \rightarrow (0, \infty)$ which satisfy the conditions in the statement of Corollary 3.16. Then the map $d_\zeta(G, G') := \|G - G'\|_\zeta^\infty$ is a translation-invariant metric on $\mathcal{G}(V)$ which once again metrizes the product topology. In fact, the following more general result is true, and the proof follows using standard topological arguments.

Proposition 3.18. *Similar to the $I = K_V$ case, define $\ell_+^p(I)$ for $p = 1, \infty$ and any subset $I \subset K_V$. Now given a partition $K_V = I_0 \coprod I_1$, as well as $\varphi \in \ell_+^1(I_0)$ and $\zeta \in \ell_+^\infty(I_1)$, define the corresponding “mixed norm” to be:*

$$d_{\varphi, \zeta}(G, G') := \|(G - G') \cap I_0\|_\varphi^1 + \|(G - G') \cap I_1\|_\zeta^\infty.$$

Then all mixed norms $\{d_{\varphi, \zeta} : I_0 \subset K_V, \varphi \in \ell_+^1(I_0), \zeta \in \ell_+^\infty(K_V \setminus I_0)\}$ are translation-invariant metrics on $\mathcal{G}(V)$ which metrize the product topology (and hence are topologically equivalent).

Note that the above theory of differentiation on $\mathcal{G}(V)$ contrasts the situation in the unlabelled setting, where graphon space is path-connected and convex, so that one directly uses Gâteaux derivatives instead of operating through a homeomorphism to \mathbb{R} . In that case it is more standard to state and prove a First Derivative Test using Gâteaux derivatives. Moreover, in the graphon setting homomorphism densities are not locally constant (as they are in $\mathcal{G}(V)$), and their derivatives have been carefully explored in joint work [DGKR] with Diao and Guillot.

Remark 3.19. Similar results (as in this section) can be obtained by using other homeomorphisms from a subset of $\mathcal{G}(V)$ onto its image in \mathbb{R} . If we fix our domain as $\mathcal{G}'(V)$, then any two such maps “differ” by a self-homeomorphism of $[0, 1] \setminus \mathbb{D}_2$.

3.4. Invariance of local extrema under choice of edge-labelling. In order to examine the local extreme values of a given function $f : \mathcal{G}(V) \rightarrow \mathbb{R}$, one approach is to proceed via the First Derivative Test on graph space. This approach consists of the following steps:

- (1) Fix a labelling of the edges, which is a bijection $\psi : K_V \rightarrow \mathbb{N}$. One advantage of the First Derivative Test as in Theorem 3.9 is that any bijection will suffice, as is explained presently.
- (2) Now compute $f'(G)$ at a point $G \neq \mathbf{0}, K_V$ via the definition, and solve the equation: $f'(G) = 0$.
- (3) To compute whether or not this is a local maximum or minimum, also use the Second Derivative Test.

A natural concern that may arise is regarding how the topological and differential structure of graph space (such as the determination of local extreme values) depends on a specific choice of vertex- or edge-labelling. Indeed, note that there is a large symmetry group that acts on $\mathcal{G}(V)$, consisting of all vertex relabellings - i.e., the permutations of V . This is parallel to the unlabelled setting of graphons, where one works with the group of all measure-preserving bijections of $[0, 1]$ (or more generally, weak isomorphisms).

In the labelled setting of $\mathcal{G}(V)$, we now study not just the permutations of V but also the larger group S_{K_V} of permutations of the edge set K_V . The first observation is that S_{K_V} leaves unchanged the topology of $\mathcal{G}(V)$, since any two labellings induce topologically equivalent metrics by (the remarks after) Proposition 2.7. Second, the determination of local extreme values is also independent of the edge-labelling. More precisely, any bijection can be chosen in the first step mentioned above. Indeed, this is clear because the concept of a local extreme point is topological in nature, so that local extrema of $f : \mathcal{G}(V) \rightarrow \mathbb{R}$ coincide under any two edge-labellings.

Given this information about the critical points of functions on graph space, a question that naturally arises is how edge-labellings influence the differential structure of graph space and functions defined on it. To answer this question we need some notation.

Definition 3.20. Define $S_\infty := \lim_{n \rightarrow \infty} S_{\psi^{-1}(\{1, \dots, n\})} = \bigcup_{n \in \mathbb{N}} S_{\psi^{-1}(\{1, \dots, n\})}$ to be the set of permutations of K_V , which fix all but finitely many edges.

Note that the set S_∞ is a proper normal subgroup of the group S_{K_V} of permutations of K_V . Moreover, once the vertex set V is labelled, every graph in $\mathcal{G}(V)$ is completely determined by the edges it contains. Thus, a function $f : \mathcal{G}(V) \rightarrow \mathbb{R}$ does not depend on a choice of edge-labelling as this is not needed to uniquely specify a graph in $\mathcal{G}(V)$. Our next result discusses the effect of S_{K_V} on the differential structure of graph space.

Theorem 3.21. Suppose $\sigma \in S_{K_V}$ (recall that $\psi : K_V \rightarrow \mathbb{N}$ is fixed). Now given a function $f : \mathcal{G}(V) \rightarrow \mathbb{R}$, define the σ -twisted derivative of f at a point $G \neq \mathbf{0}, K_V$ via:

$$f'_\sigma(G) := \lim_{G_1 \rightarrow G, G_1 \in \mathcal{G}'(V)} \frac{f(G_1) - f(G)}{\|G_1\|_{\sigma \circ \psi, 2} - \|G\|_{\sigma \circ \psi, 2}}.$$

Then the automorphisms in S_{K_V} preserving the differential structure of graph space are precisely S_∞ . More precisely, if $\sigma \in S_\infty$ and $f'(G)$ exists, then $f'_\sigma(G)$ exists and equals $f'(G)$. If on the other hand $\sigma \in S_{K_V} \setminus S_\infty$, $G \in \mathcal{G}'(V)$, and $f'(G) \neq 0$, then $f'_\sigma(G)$ does not exist.

In particular, a stronger statement holds than the topological one discussed above - namely, not merely the critical points, but the derivative itself remains invariant under the family S_∞ of eventually constant permutations of edge-labellings (but not under other permutations).

Proof. In this proof we will freely identify S_{K_V} with $S_{\mathbb{N}}$ via the bijection ψ . Suppose $\sigma \in S_{K_V} = S_{\mathbb{N}}$ fixes all $n > N$ for some $N > 0$. One can then show that

$$\|G - G_1\|_{\psi, 2} < 2^{-N} \iff \|G - G_1\|_{\sigma \circ \psi, 2} < 2^{-N}. \quad (3.22)$$

Also note that in this case the smallest label of an edge in $G - G_1 = G \Delta G_1$ under either ψ or $\sigma \circ \psi$ is at least $N + 1$. Therefore,

$$0 \neq \|G_1\|_{\psi,2} - \|G\|_{\psi,2} = \|G_1\|_{\sigma \circ \psi,2} - \|G\|_{\sigma \circ \psi,2},$$

if G_1 is “close enough” (in the φ_2 -metric induced by either ψ or $\sigma \circ \psi$) to G . It follows that $f'(G) = f'_\sigma(G)$ if either derivative exists.

Now suppose $f'(G)$ exists and is nonzero for some $G \in \mathcal{G}'(V)$ and $f : \mathcal{G}(V) \rightarrow \mathbb{R}$, and $f'_\sigma(G)$ exists for some $\sigma \in S_{K_V}$. Since $f'_\sigma(G)$ exists, then so does the limit

$$\frac{f'_\sigma(G)}{f'(G)} = \lim_{n \rightarrow \infty} \frac{\|G \Delta \{\psi^{-1}(n)\}\|_{\psi,2} - \|G\|_{\psi,2}}{\|G \Delta \{\psi^{-1}(n)\}\|_{\sigma \circ \psi,2} - \|G\|_{\sigma \circ \psi,2}} = \lim_{n \rightarrow \infty} \frac{2^{-n}}{2^{-\sigma(n)}} = \lim_{n \rightarrow \infty} 2^{\sigma(n)-n}.$$

Note that the sequence $\sigma(n) - n$ is integer-valued. Thus if the above limit is at most $1/2$, then there exists $N > 0$ such that $\sigma(n) - n \geq 1$ for all $n > N$. But then the bijection $\sigma : \mathbb{N} \rightarrow \mathbb{N}$ maps a subset of $\{1, \dots, N\}$ onto $\{1, \dots, N+1\}$, which is impossible.

Therefore the above limit is equal to 2^{n_0} for some $n_0 \geq 0$. Hence there exists $N > 0$ such that $\sigma(n) - n = n_0$ for all $n > N$. Now if $n_0 < 0$, then σ maps $\{1, \dots, N+n_0\}$ onto a subset of $\{1, \dots, N\}$, which is impossible. The only remaining case is that $n_0 = 0$, i.e., $\sigma \in S_\infty$. \square

Given Theorem 3.21, it is natural to ask when an automorphism $\sigma \in S_{K_V}$ preserves (the derivative at) critical points of f . The following result provides partial information along these lines.

Proposition 3.23. *Suppose $f : \mathcal{G}(V) \rightarrow \mathbb{R}$ is such that $f'(G) = 0$. Suppose there exists a sequence $G_n \rightarrow G$ in $\mathcal{G}'(V)$ such that $f(G_n) \neq f(G)$ and $G_n \setminus G$ is finite for all n . Then there exists $\sigma \in S_{K_V}$ such that $f'_\sigma(G) \neq 0$.*

Proof. We first define subsequences n_k, m_k, m'_k of \mathbb{N} as follows: set $E_n := G_n \setminus G$, $m_1 := 0$, and $n_1 := 1$. Now given n_k , define

$$m'_k := \max \psi(E_{n_k}), \quad m_{k+1} := \min([m'_k + 1, \infty) \cap \mathbb{N}) \setminus \psi(G).$$

Next, define n_{k+1} to be the least n such that $\min \psi(E_n) > m_{k+1}$. Now we define $t_0 := 0$ and an auxiliary sequence $0 < t_1 < t_2 < \dots \in \mathbb{N}$ as follows:

$$t_k := 1 + \max(t_{k-1} + m_k - m_{k-1}, \frac{-\ln |f(G_{n_k}) - f(G)|}{\ln 2}).$$

Now define the permutation $\sigma_{\mathbb{N}} : \mathbb{N} \rightarrow \mathbb{N}$ as follows: $\sigma_{\mathbb{N}}$ sends $n \in (m_k, m_{k+1})$ to $n + t_k - m_k$ for all $k \in \mathbb{N}$, and is an order-preserving bijection from $\{m_2, m_3, \dots\}$ onto $\mathbb{N} \setminus \coprod_{k \in \mathbb{N}} (t_k, t_k + m_{k+1} - m_k)$. Finally, define $\sigma : K_V \rightarrow K_V$ via: $\sigma := \psi^{-1} \circ \sigma_{\mathbb{N}} \circ \psi$. We then claim that $f'_\sigma(G) \neq 0$. More precisely, note that for all k ,

$$|\|G_{n_k}\|_{\sigma \circ \psi,2} - \|G\|_{\sigma \circ \psi,2}| \leq 2^{-(t_k+1)} + 2^{-(t_k+2)} + \dots = 2^{-t_k} < |f(G_{n_k}) - f(G)|.$$

It follows that

$$\lim_{k \rightarrow \infty} \frac{f(G_{n_k}) - f(G)}{\|G_{n_k}\|_{\sigma \circ \psi,2} - \|G\|_{\sigma \circ \psi,2}} \neq 0,$$

which concludes the proof. \square

4. THE LIMITING EDGE DENSITY OF A COUNTABLE GRAPH

Thus far we have explored the space of all labelled graphs in terms of its topology and differential structure. We now proceed to draw further parallels to the unlabelled setting which are not directly related to the theory of differentiation developed above. Recall that the notion of homomorphism density has a labelled analogue via homomorphism indicators, and these were explored in detail in Section 2.3. In the final section of this paper, we introduce and briefly examine an alternate approach to studying homomorphism densities in the labelled setting: namely, in a limiting sense.

Definition 4.1. Henceforth fix a countable vertex set V , as well as a bijection $\xi : V \rightarrow \mathbb{N}$ which labels the vertices. Given a graph $G \in \mathcal{G}(V)$ and $n \in \mathbb{N}$, define $G_V[n]$ to be the finite subgraph of G induced on the vertices $\xi^{-1}(1), \dots, \xi^{-1}(n)$.

Given a finite simple graph H and a finite simple labelled graph G , denote by $\text{ind}(H, G)$ the number of embeddings of H into G as an induced subgraph. Now define the corresponding *induced homomorphism density* to equal $t_{\text{ind}}(H, G) := \text{ind}(H, G) \cdot (|V(G)| - |V(H)|)! / |V(G)|!$.

Next, if $G \in \mathcal{G}(V)$, then define the *limiting induced homomorphism density of H in G* to equal

$$t_{\text{ind}}(H, G) := \lim_{n \rightarrow \infty} t_{\text{ind}}(H, G_V[n]),$$

if this limit exists. Also define $S(H, G)$ to be the set of accumulation points of the sequence $t_{\text{ind}}(H, G_V[n])$.

We define and study the sets $S(H, G)$ because it is not always the case that limiting induced homomorphism densities converge. Thus we initiate the study of (the sets of) limiting homomorphism densities in this section. We will focus on the *limiting edge density* of a countable graph, which is a useful summary statistic. Given a finite graph G on n vertices, the edge density is precisely the number of edges in it, divided by the total number of possible edges - namely, $e(G) := |E(G)| / \binom{n}{2}$. It is now natural to ask questions on the limiting edge density. For instance, if the number of vertices is a fixed finite number n , what is the probability mass function satisfied by the edge density on all labelled graphs on n vertices? Is there a limit of these probability distributions as more and more nodes are added to the graph - i.e., as $n \rightarrow \infty$? To answer the first of these questions, note that there are $2^{\binom{n}{2}}$ possible labelled graphs on n vertices, and the number of edges in a graph follows a binomial distribution. Thus if e_n denotes the edge density of a random graph on n vertices, then

$$\mathbb{P}(e_n = \binom{n}{2}^{-1} m) = \binom{\binom{n}{2}}{m} 2^{-\binom{n}{2}}.$$

In the limit as $n \rightarrow \infty$, these edge densities converge almost everywhere by the Strong Law of Large Numbers to $1/2$, since e_n is the average of $\binom{n}{2}$ i.i.d. Bernoulli($\frac{1}{2}$) random variables.

Thus, we take a closer look at edge densities. The main result in this section studies the set of possible edge densities that can arise for countable labelled graphs.

Theorem 4.2. *Suppose H is a finite simple graph and $G \in \mathcal{G}(V)$. Then $S(H, G)$ is a closed and nonempty subset of $[0, 1]$. If $H = K_2$ is the complete graph on 2 vertices, then $S(K_2, G)$ is a closed subinterval of $[0, 1]$. Conversely, given any nonempty closed subinterval $[a, b] \subset [0, 1]$, there exists $G \in \mathcal{G}(V)$ such that $S(K_2, G) = [a, b]$.*

The technical heart of the proof of Theorem 4.2 lies in the following result.

Theorem 4.3. *Fix an enumeration $\xi : V \rightarrow \mathbb{N}$ of the vertices in V .*

- (1) *For every countable graph $G \in \mathcal{G}(V)$, there exists a subsequence $n_1 < n_2 < \dots$ in \mathbb{N} , such that $e(G_V[n_k])$ converges as $n \rightarrow \infty$ (to a limit in $[0, 1]$).*
- (2) *The previous statement is “sharp” in the sense that for any finite set of points $0 \leq e_1 < \dots < e_m \leq 1$ with $m > 1$, there exists a countable graph $G \in \mathcal{G}(V)$ and subsequences $n_{i1} < n_{i2} < \dots < n_{im} \in \mathbb{N}$, such that*

$$\lim_{k \rightarrow \infty} e(G_V[n_{ik}]) = e_i, \quad \forall 1 \leq i \leq m,$$

and all limiting edge densities of G lie in $[e_1, e_m]$.

- (3) *Given $e \in [0, 1]$, there exists $G \in \mathcal{G}(V)$ such that $e(G_V[n]) \rightarrow e$.*

Proof.

- (1) For all n , $e(G_V[n]) \in [0, 1]$. Hence there exists a convergent subsequence $e(G_V[n_k])$ as desired.

- (2) We first claim that the following holds: given $0 \leq p_0 < p_1 \leq 1$, $0 < \epsilon < (p_1 - p_0)/2$, and a finite graph G with $e(G) = p_i$, there exists a finite graph $H \supset G$ such that $|e(H) - p_{1-i}| < \epsilon$, and such that for each “intermediate” graph H' (i.e., $|V(G)| < |V(H')| < |V(H)|$), $e(H') \in [p_0, p_1]$.

We show only the claim for $i = 0$; the other case is proved similarly. If G has n_1 vertices, then define:

$$n_2 := 1 + \max(\sqrt{2/\epsilon}, n_1\sqrt{p_1/(p_0 + \epsilon)}, n_1\sqrt{(1 - p_0)/(1 - p_1 + \epsilon)}).$$

Note that $n_2 > n_1$ as desired. We now construct a graph $H \supset G$ on n_2 vertices as follows: first attach $n_2 - n_1$ vertices to G . If no extra edges are added, then the resulting graph has edge density at most $e(G) = p_0 < p_1$. If all extra edges (i.e., all edges that are not between vertices in $V(G)$) are added, then the resulting graph has edge density

$$\binom{n_2}{2}^{-1} \left[p_0 \binom{n_1}{2} + \binom{n_2}{2} - \binom{n_1}{2} \right] = 1 - \frac{n_1(n_1 - 1)(1 - p_0)}{n_2(n_2 - 1)} \geq 1 - \frac{n_1^2(1 - p_0)}{(n_2 - 1)^2} \geq p_1 - \epsilon.$$

Thus we attach a suitable number of edges among the $\binom{n_2}{2} - \binom{n_1}{2}$ extra edges. At each stage, the edge density is increasing, so it is at least p_0 . Finally, observe that it is possible to increase the edge density until it lies in $(p_1 - \epsilon, p_1]$, since adding an edge among the n_2 vertices changes the edge density by $\binom{n_2}{2}^{-1} \leq ((n_2 - 1)^2/2)^{-1} < \epsilon$. But then the edge densities of all “intermediate” graphs lie in $[p_0, p_1]$, and the claim is proved.

We now show the result given the above claim. To do so, define $\epsilon_0 := \frac{1}{2} \min_{0 < i < m} (e_{i+1} - e_i)$, and begin with a graph G_{11} with edge density in $[e_1, e_1 + \epsilon_0) \subset (e_1 - \min(1, \epsilon_0), e_1 + \min(1, \epsilon_0))$. This is easy to achieve by choosing integers $0 < r < s$ such that $|e_1 - \binom{s}{2}^{-1}r| < \min(1, \epsilon_0)$. Set $n_{11} := |V(G_{11})|$.

Now proceed inductively as follows: suppose we have constructed the G_{ik} on n_{ik} vertices with edge density in $(e_i - \min(1/k, \epsilon_0), e_i + \min(1/k, \epsilon_0)) \cap [e_1, e_m]$, for some $1 \leq i \leq m$ and $k \in \mathbb{N}$. If $i < m$, then apply the claim to construct a graph $G_{i+1,k} \supset G_{ik}$, with increased edge density: $e(G_{i+1,k}) \in (e_{i+1} - \min(1/k, \epsilon_0), e_{i+1}]$. Now define $n_{i+1,k} := |V(G_{i+1,k})|$. Similarly, if $i = m$, then apply the claim to construct a graph $G_{1,k+1} \supset G_{m,k}$, with reduced edge density: $e(G_{1,k+1}) \in [e_1, e_1 + \min(1/(k+1), \epsilon_0))$. Now define $n_{1,k+1} := |V(G_{1,k+1})|$. This construction clearly proves the result, once we observe that by the above claim in the proof, the edge densities always stay inside $[e_1, e_m]$.

- (3) We first record a fact which is useful later in this paper. Namely, suppose G is a graph with n vertices and edge density e . Then adding one more vertex and no additional edges yields a graph with edge density

$$\binom{n+1}{2}^{-1} \binom{n}{2} e = \frac{n-1}{n+1} e,$$

while adding all additional edges yields a graph with edge density

$$\binom{n+1}{2}^{-1} \left(\binom{n}{2} e + \binom{n+1}{2} - \binom{n}{2} \right) = 1 - \frac{n-1}{n+1} (1 - e) = \frac{n-1}{n+1} e + \frac{2}{n+1}.$$

Thus for all graphs $G \in \mathcal{G}(V)$ and $n \in \mathbb{N}$,

$$\frac{n-1}{n+1} e(G_V[n]) \leq e(G_V[n+1]) \leq \frac{n-1}{n+1} e(G_V[n]) + \frac{2}{n+1}. \quad (4.4)$$

Now given $e \in [0, 1]$, if $e = 0$ or 1 then we choose $G = \emptyset$ or K_V to obtain the desired countable graph with edge density e . Otherwise suppose $e \in (0, 1)$ and set $G_2 := K_2$. Then $|e(G_2) - e| < \binom{2}{2}^{-1} = 1$. We now inductively construct an increasing sequence of graphs G_n such that $|e - e(G_n)| < \binom{n}{2}^{-1}$ for all $n \geq 2$; this shows that $\lim_{n \rightarrow \infty} e(G_n) = e$ as desired.

Given G_n for $1 < n \in \mathbb{N}$ such that $|e(G_n) - e| < \binom{n}{2}^{-1}$, add a node to G_n together with a certain number of additional edges (which are specified presently) not between the nodes of G_n . By Equation (4.4), this yields a graph with edge density between $a := \frac{n-1}{n+1}e(G_n)$ and $b := \frac{n-1}{n+1}e(G_n) + \frac{2}{n+1}$. But now compute that

$$\begin{aligned} a &= \frac{n-1}{n+1}e(G_n) < \frac{n-1}{n+1}\left(e + \binom{n}{2}^{-1}\right) = \frac{n-1}{n+1}e + \binom{n+1}{2}^{-1} < e + \binom{n+1}{2}^{-1}, \\ b &> \frac{n-1}{n+1}\left(e - \binom{n}{2}^{-1}\right) + \frac{2}{n+1} = \frac{2 + (n-1)e}{n+1} - \binom{n+1}{2}^{-1} > e - \binom{n+1}{2}^{-1}. \end{aligned}$$

Now we consider various cases. If $a > e - \binom{n+1}{2}^{-1}$ or $b < e + \binom{n+1}{2}^{-1}$, then we add no or all edges connecting vertex $n+1$ to G_n , respectively. This yields G_{n+1} with edge density in $(e - \binom{n+1}{2}^{-1}, e + \binom{n+1}{2}^{-1})$ as desired.

The remaining case is when $a \leq e - \binom{n+1}{2}^{-1} < b \leq e + \binom{n+1}{2}^{-1}$. In this case it is possible to add an integer multiple (say k) of $\binom{n+1}{2}^{-1}$ to a to obtain a number in $(e - \binom{n+1}{2}^{-1}, e + \binom{n+1}{2}^{-1})$ as desired. Now construct G_{n+1} by connecting the additional vertex $n+1$ to precisely k vertices in G_n . This concludes the proof by induction on n , with $e(G_n) \rightarrow e$. \square

It is now possible to prove the main result of this section.

Proof of Theorem 4.2. First fix a finite simple graph H . Then $S(H, G)$ is nonempty because for all $n \in \mathbb{N}$, $t_{\text{ind}}(H, G_V[n]) \in [0, 1]$ and hence there exists a convergent subsequence $t_{\text{ind}}(H, G_V[n_k])$ as desired. Next, suppose e is an accumulation point of $S(H, G)$, and $e_1 < e_2 < \dots$ converges to $e \in [0, 1]$, with $e_l \in S(H, G)$ for all $l \in \mathbb{N}$. Thus for all $l \in \mathbb{N}$, there exists an infinite subsequence $n_{l1} < n_{l2} < \dots$ in \mathbb{N} such that $t_{\text{ind}}(H, G_V[n_{lk}]) \rightarrow e_l$ as $k \rightarrow \infty$. Now set $n'_0 := 0$, and given n'_{l-1} for $l \in \mathbb{N}$, choose k_l such that

$$n_{lk_l} > n'_{l-1}, \quad |t_{\text{ind}}(H, G_V[n_{lk_l}]) - e_l| < \frac{1}{l}.$$

Now define $n'_l := n_{l, k_l}$. Then the n'_l form an increasing subsequence in \mathbb{N} such that

$$|t_{\text{ind}}(H, G_V[n'_l]) - e| \leq |t_{\text{ind}}(H, G_V[n'_l]) - e_l| + (e - e_l) < \frac{1}{l} + (e - e_l).$$

We conclude that $e \in S(H, G)$. A similar argument in the case when $e_1 > e_2 > \dots$ converges to $e \in [0, 1]$ now concludes the proof and shows that $S(H, G) \subset [0, 1]$ is closed for all H .

We now show that $S(K_2, G)$ is a closed interval. Given $e \in (\inf S(K_2, G), \sup S(K_2, G))$, fix any sequence $n_1 < n_2 < \dots$ in \mathbb{N} such that

$$\begin{aligned} \lim_{k \rightarrow \infty} e(G_V[n_{2k-1}]) &= \inf S(K_2, G) \neq \sup S(K_2, G) = \lim_{k \rightarrow \infty} e(G_V[n_{2k}]), \\ e(G_V[n_{2k-1}]) &< e < e(G_V[n_{2k}]) \quad \forall k \in \mathbb{N}. \end{aligned}$$

By Equation (4.4), note that for all $n \in \mathbb{N}$, we have that $e(G_V[n+1]) \leq e(G_V[n]) + 2/(n+1)$. Now given n_{2k-1} , add one vertex at a time under the given enumeration, so that the edge density increases with each additional vertex by at most $2/(n+1) \leq 2/(n_{2k-1}+1)$. Now choose $n'_k \in [n_{2k-1}, n_{2k}]$ such that

$$|e(G_V[n'_k]) - e| < \frac{2}{n_{2k-1}+1}, \quad \forall k \in \mathbb{N}.$$

This immediately implies that (the n'_k are increasing and) $\lim_{k \rightarrow \infty} e(G_V[n'_k]) = e$, as desired.

To prove the last assertion given $0 \leq a \leq b \leq 1$, note that if $a = b$ then we are done by the last part of Theorem 4.3. If $a < b$ instead, then apply another part of Theorem 4.3, with $m = 2$ and

$0 \leq e_i := a < b =: e_s \leq 1$, via the construction given in the proof. Thus we conclude that both e_i, e_s are limiting edge densities of G , but no numbers in $[0, e_i) \cup (e_s, 1]$ are. The result now follows from the above analysis in this proof. \square

Concluding remarks. We conclude by noting that this paper systematically develops a rigorous foundation and mathematical theory for the analysis of labelled graphs. The motivation for this endeavor comes from real-world phenomena, and as discussed above, the model of graph space discussed in this paper has a rich structure, allowing us to study topology, analysis, and differentiation on $\mathcal{G}(V)$. In subsequent work [KR], we use these properties to study measure theory on graph space $\mathcal{G}(V)$, with the goal of developing and exploring Lebesgue-type integration and probability theory on it.

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REFERENCES

- [AKM] M. Axenovich, A. Kézdy, and R. Martin, *On the editing distance of graphs*, Journal of Graph Theory **58** (2008), no. 2, 123–138.
- [BJR] B. Bollobás, S. Janson, and O. Riordan, *Sparse random graphs with clustering*, Random Structures & Algorithms **38**, no. 3 (2011), 269–323.
- [BR] B. Bollobás and O. Riordan, *Metrics for sparse graphs*, Surveys in Combinatorics 2009, London Math. Soc. Lecture Note Series **365**, S. Huczynska, J.D. Mitchell, and C.M. Roney-Dougal eds. (2009), 211–287.
- [BCCZ1] C. Borgs, J. Chayes, H. Cohn, and Y. Zhao, *An L^p theory of sparse graph convergence I: limits, sparse random graph models, and power law distributions*, preprint (2014), <http://arxiv.org/abs/1401.2906>.
- [BCCZ2] C. Borgs, J. Chayes, H. Cohn, and Y. Zhao, *An L^p theory of sparse graph convergence II: LD convergence, quotients, and right convergence*, preprint (2014), <http://arxiv.org/abs/1408.0744>.
- [BCLSV] C. Borgs, J. Chayes, L. Lovász, V.T. Sós, and K. Vesztegombi, *Convergent sequences of dense graphs I: Subgraph frequencies metric properties, and testing*, Advances in Mathematics **219** (2008), no. 6, 1801–1851.
- [Cam] P.J. Cameron, *Cyclic automorphisms of a countable graph and random sum-free sets*, Graphs and Combinatorics **1** (1985), no. 1, 129–135.
- [DJK1] Z. Daróczy, A. Járαι, and I. Kátai, *Interval filling sequences*, Annales Univ. Eötvös L. Sectio Computatorica **6** (1985), 53–63.
- [DJK2] Z. Daróczy, A. Járαι, and I. Kátai, *Intervallfüllende Folgen und volladditive Funktionen*, Acta Sci. Math. Szeged **50** (1986), 337–350.
- [DGKR] P. Diao, D. Guillot, A. Khare, and B. Rajaratnam, *Differential calculus on graphon space*, preprint (2014), <http://arxiv.org/abs/1403.3736>.
- [FK] A. Frieze and R. Kannan, *Quick approximation to matrices and applications*, Combinatorica **19** (1999), no. 1, 175–220.
- [KR] A. Khare and B. Rajaratnam, *Integration and tail estimates on the space of countable graphs*, work in progress.
- [Lo] L. Lovász, *Large networks and graph limits*, Colloquium Publications **60**, American Mathematical Society, Providence, RI, 2012.
- [LS1] L. Lovász and B. Szegedy, *Limits of dense graph sequences*, Journal of Combinatorial Theory, Series B **96** (2006), no. 6, 933–957.

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